

=&gt; b reg

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STRUCTURE FILE UPDATES: 15 AUG 2007 HIGHEST RN 944769-12-4  
 DICTIONARY FILE UPDATES: 15 AUG 2007 HIGHEST RN 944769-12-4

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

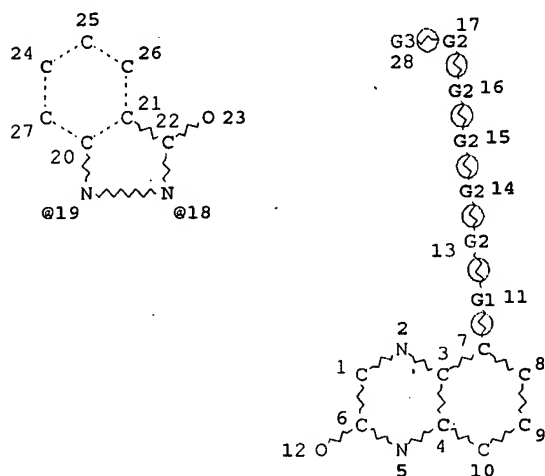
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REGISTRY includes numerically searchable data for experimental and  
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 experimental property data in the original document. For information  
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=&gt; d que sta 17

L1 STR



VAR G1=O/N  
 VAR G2=C/N/O  
 VAR G3=18/19  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE  
 L7 218 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 472 ITERATIONS  
 SEARCH TIME: 00.00.01

218 ANSWERS

=&gt; b hcap

FILE 'HCAPLUS' ENTERED AT 16:12:38 ON 16 AUG 2007  
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FILE COVERS 1907 - 16 Aug 2007 VOL 147 ISS 8  
FILE LAST UPDATED: 15 Aug 2007 (20070815/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d bib abs hitrn fhitr 112 tot

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:390252 HCAPLUS

DN 140:406823

TI Preparation of quinoxaline derivatives as Cdk inhibitors

IN Hirai, Hiroshi; Kawanishi, Nobuhiko; Hirose, Masaaki; Sugimoto, Tetsuya; Kamijyo, Kaori; Shibata, Jun; Masutani, Kouta

PA Banyu Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 306 pp.

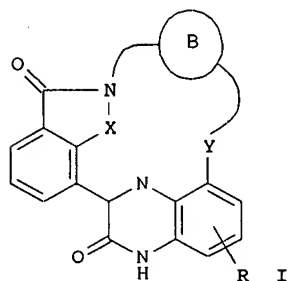
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2004039809	A1	20040513	2003WO-JP13707	20031027 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA---2503663	A1	20040513	2003CA-2503663	20031027 <--
	AU2003275681	A1	20040525	2003AU-0275681	20031027 <--
	EP---1557418	A1	20050727	2003EP-0758937	20031027 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US2006019959	A1	20060126	2005US-0532677	20050615 <--
PRAI	2002JP-0313588	A	20021029 <--		
	2003WO-JP13707	W	20031027 <--		
OS	MARPAT 140:406823				
GI					



AB The title compds. I [X is NH, S, or the like; Y is O or the like; ring B is -B1(B1')B2(B2')B3(B3')B4(B4')B5(B5')-, etc.; B1 - B5 are each independently CH, N, or the like; and B1' - B5' are each independently hydrogen or the like; and R is hydrogen, lower alkyl, or the like] are prepared. Compds. of this invention in vitro showed IC50 values of 1.6 nM to 34 nM against cyclin D2-cdk4.

IT 688806-23-7P 688806-24-8P 688806-25-9P  
 688806-65-7P 688806-66-8P 688806-67-9P  
 688806-68-0P 688806-69-1P 688806-70-4P  
 688806-71-5P 688806-72-6P 688806-73-7P  
 688806-74-8P 688806-75-9P 688806-76-0P  
 688806-77-1P 688806-78-2P 688806-79-3P  
 688806-80-6P 688806-81-7P 688806-82-8P  
 688806-83-9P 688806-84-0P 688806-85-1P  
 688806-86-2P 688806-87-3P 688806-88-4P  
 688806-91-9P 688806-92-0P 688806-93-1P  
 688806-95-3P 688807-02-5P 688807-03-6P  
 688807-04-7P 688807-05-8P 688807-06-9P  
 688807-07-0P 688807-08-1P 688807-10-5P  
 688807-12-7P 688807-13-8P 688807-15-0P  
 688807-17-2P 688807-19-4P 688807-20-7P  
 688807-21-8P 688807-23-0P 688807-25-2P  
 688807-27-4P 688807-28-5P 688807-29-6P  
 688807-31-0P 688807-33-2P 688807-34-3P  
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 688807-41-2P 688807-43-4P 688807-45-6P  
 688807-47-8P 688807-49-0P 688807-51-4P  
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 688807-59-2P 688807-61-6P 688807-63-8P  
 688807-65-0P 688807-67-2P 688807-69-4P  
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 688807-83-2P 688807-84-3P 688807-85-4P  
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 688807-92-3P 688807-93-4P 688807-94-5P  
 688807-95-6P 688807-96-7P 688807-97-8P  
 688807-98-9P 688807-99-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinoxaline derivs. as Cdk inhibitors)

IT 688808-28-8P 688808-29-9P 688808-86-8P  
 688808-87-9P 688808-88-0P 688808-89-1P  
 688808-90-4P 688809-03-2P 688809-18-9P  
 688809-19-0P 688809-20-3P 688809-21-4P  
 688809-25-8P 688809-26-9P 688809-27-0P  
 688809-32-7P 688809-33-8P 688809-34-9P  
 688809-35-0P 688809-36-1P 688809-37-2P  
 688809-38-3P 688809-39-4P 688809-40-7P  
 688809-41-8P 689283-08-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinoxaline derivs. as Cdk inhibitors)

IT 688806-23-7P

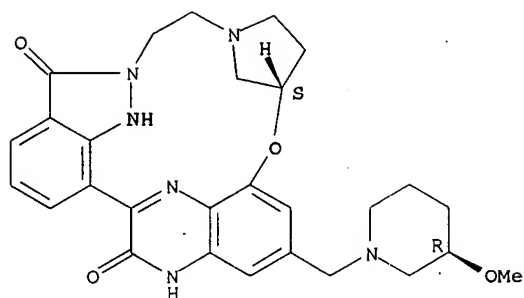
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinoxaline derivs. as Cdk inhibitors)

RN 688806-23-7 HCAPLUS

CN 5H,10H-17,19-(Iminomethano)-4,6:9,12-dimethanodibenz[b,f][1,4,8,9,12]oxate  
 traazacyclopentadecine-20,23-dione, 7,8,11,12-tetrahydro-15-[[[(3R)-3-methoxy-1-piperidinyl]methyl]-, monohydrochloride, (12S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

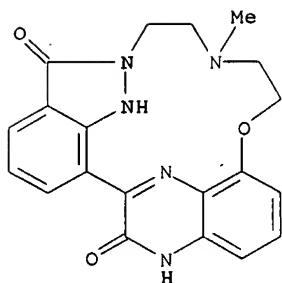


● HCl

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr l13 tot

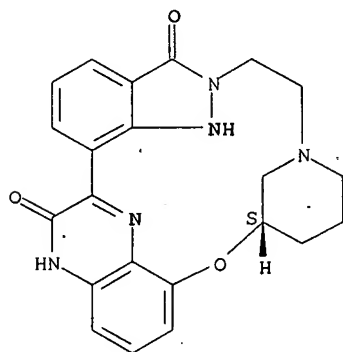
L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN  
AN 2006:874447 HCAPLUS  
DN 145:448576  
TI Structure-based drug design of a highly potent CDK1,2,4,6 inhibitor with  
novel macrocyclic quinoxaline-2-one structure  
AU Kawanishi, Nobuhiko; Sugimoto, Tetsuya; Shibata, Jun; Nakamura, Kaori;  
Masutani, Kouta; Ikuta, Mari; Hirai, Hiroshi  
CS Department of Medicinal Chemistry, Banyu Tsukuba Research Institute in  
collaboration with Merck Research Laboratories, Tsukuba, Ibaraki,  
300-2611, Japan  
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(19), 5122-5126  
CODEN: BMCLE8; ISSN: 0960-894X  
PB Elsevier Ltd.  
DT Journal  
LA English  
OS CASREACT 145:448576  
AB The design of a novel series of cyclin-dependent kinase (CDK) inhibitors  
containing a macrocyclic quinoxaline-2-one is reported. Structure-based drug  
design and optimization from the starting point of diarylurea 2, which we  
previously reported as a moderate CDK1,2,4,6 inhibitor, led to the  
discovery of potent CDK1,2,4,6 inhibitor that were suitable for iv  
administration for in vivo study.  
IT 913375-38-9 913375-39-0 913375-40-3  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
(structure-based drug design of highly potent CDK1,2,4,6 inhibitor with  
macrocyclic quinoxalinone structure)  
RN 913375-38-9 HCAPLUS  
CN 7H-16,18-(Iminomethano)-4,6-methano-5H-dibenz[i,m][1,4,7,8,12]oxatetraazac  
yclotetradecine-19,21-dione, 8,9,10,11-tetrahydro-9-methyl-,  
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

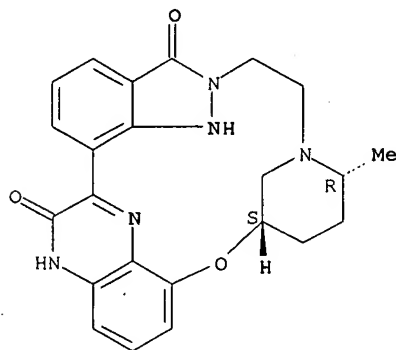
RN 913375-39-0 HCAPLUS  
 CN 18,20-(iminomethano)-4,6:9,13-dimethano-5H-dibenz[b,f][1,4,8,9,12]oxatetraazacyclohexadecine-21,24-dione, 7,8,10,11,12,13-hexahydro-, (13S)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



RN 913375-40-3 HCAPLUS  
 CN 18,20-(iminomethano)-4,6:9,13-dimethano-5H-dibenz[b,f][1,4,8,9,12]oxatetraazacyclohexadecine-21,24-dione, 7,8,10,11,12,13-hexahydro-10-methyl-, (10R,13S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> b uspatall  
 FILE 'USPATFULL' ENTERED AT 16:13:03 ON 16 AUG 2007  
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FILE 'USPAT2' ENTERED AT 16:13:03 ON 16 AUG 2007  
CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs fhitr 114 tot

L14 ANSWER 1 OF 1 USPATFULL on STN  
AN 2006:22125 USPATFULL  
TI Novel quinoxalinone derivatives  
IN Hirai, Hiroshi, c/o Banyu Pharmaceutical Co., Ltd., Tsukuba Research  
Institute, 3, Okubo, Tsukuba-shi, Ibaraki, JAPAN 300-2611  
Kawanishi, Nobuhiko, Tsukuba, JAPAN  
Hirose, Masaaki, Tsukuba, JAPAN  
Sugimoto, Tetsuya, Tsukuba, JAPAN  
Kamijyo, Kaori, Tsukuba, JAPAN  
Shibata, Jun, Tsukuba, JAPAN  
Masutani, Kouta, Tsukuba, JAPAN  
PA Banyu Pharmaceutical Co., Ltd. Tsukuba Research Institute, Ibaraki,  
JAPAN, 300-2611 (non-U.S. corporation)  
PI US-20060019959 A1 20060126  
AI 2003US-000532677 A1 20031027 (10)  
2003WO-JP00013707 20031027  
20050615 PCT 371 date  
PRAI 2002JP-000313588 20021029  
DT Utility  
FS APPLICATION  
LREP WENDEROTH, LIND & PONACK, L.L.P., 2033 K STREET N. W., SUITE 800,  
WASHINGTON, DC, 20006-1021, US  
CLMN Number of Claims: 18  
ECL Exemplary Claim: 1  
DRWN No Drawings  
LN.CNT 6099

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A quinoxalinone derivative of the formula (I): ##STR1## or a  
pharmaceutically acceptable salt or ester thereof, wherein; X is NH, S  
or the like; Y is O or the like; the partial structure ##STR2##  
is, for example, the formula: ##STR3##

B.sub.1, B.sub.2, . . . , B.sub.n-1 and B.sub.n, (in which n is 4, 5 or 6) are  
each independently CH, N or the like;  
B'.sub.1, B'.sub.2, . . . , B'.sub.n-1 and B'.sub.n (in which n is 4, 5 or 6)  
are each independently hydrogen or the like; and R is hydrogen, lower  
alkyl or the like.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

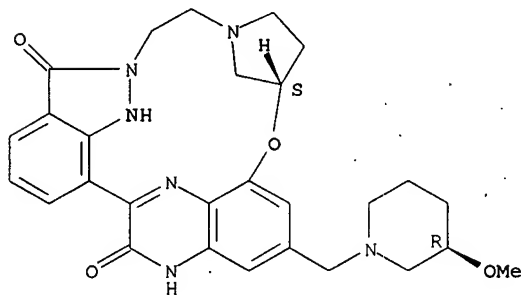
IT 688806-23-7P

(préparation of quinoxaline derivs. as Cdk inhibitors)

RN 688806-23-7 USPATFULL

CN 5H,10H-17,19-(Iminomethano)-4,6:9,12-dimethanodibenz[b,f][1,4,8,9,12]oxate  
traazacyclopentadecine-20,23-dione, 7,8,11,12-tetrahydro-15-[(3R)-3-  
methoxy-1-piperidinyl]methyl-, monohydrochloride, (12S)- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



● HCl

=> d his

(FILE 'HOME' ENTERED AT 15:39:39 ON 16 AUG 2007)

FILE 'REGISTRY' ENTERED AT 15:39:50 ON 16 AUG 2007

L1 STR

FILE 'HCAPLUS' ENTERED AT 15:51:03 ON 16 AUG 2007

L2 1 US20060019959/PN OR (US2005-532677 OR JP2002-313588 OR WO2003-J

FILE 'REGISTRY' ENTERED AT 15:52:49 ON 16 AUG 2007

FILE 'HCAPLUS' ENTERED AT 15:52:49 ON 16 AUG 2007

L3 TRA L2 1- RN : 511 TERMS

FILE 'REGISTRY' ENTERED AT 15:52:50 ON 16 AUG 2007

L4 511 SEA L3

L5 282 L4 AND NR>=4

L6 9 L1

L7 218 L1 FULL

SAV TEM L7 J677C1/A

L8 121 L7 AND L4

L9 97 L7 NOT L8

FILE 'HCAOLD' ENTERED AT 16:07:47 ON 16 AUG 2007

L10 0 L7

FILE 'HCAPLUS' ENTERED AT 16:08:02 ON 16 AUG 2007

L11 2 L7

L12 1 L11 AND L2

L13 1 L11 NOT L12

FILE 'USPATFULL, USPAT2' ENTERED AT 16:10:40 ON 16 AUG 2007

L14 1 L7

FILE 'BIOSIS' ENTERED AT 16:11:29 ON 16 AUG 2007

L15 0 L7

FILE 'MEDLINE' ENTERED AT 16:11:37 ON 16 AUG 2007

L16 0 L7

FILE 'EMBASE' ENTERED AT 16:11:42 ON 16 AUG 2007

L17 0 L7

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